Office of Science
U.S. DEPARTMENT OF ENERGY

Advanced Scientific Computing Research

FY2005 Accomplishments

Leadership Class Computing

Center for Computational Sciences

J. Nichols,* Oak Ridge National Laboratory

Summary

The Center for Computational Sciences (CCS) at the Oak Ridge National Laboratory was established in 1992 and in 2004 was designated by the Secretary of Energy as the Leadership Computing Facility for the nation, providing a resource 100 times more powerful than current capabilities.

The Leadership Computing Facility (LCF) is building the world's most powerful supercomputer for unclassified scientific research. The facility provides researchers an unparalleled environment for new discoveries that will dramatically impact the nation's ability to produce a secure energy economy and increase mankind's understanding of our world, from the molecules in the air we breathe, to the birth and death of the stars in the sky. As a designated User Facility, the LCF

- delivers leadership-class computing for science and engineering
- focuses on grand challenge science and engineering applications
- procures largest-scale computer systems (beyond vendors design point) and develop high-end operational and application software
- educates and trains next generation computational scientists

Today, the computing resources of the Leadership Computing Facility are among the fastest in the world, able to perform more than 40 trillion calculations per second. The Cray X1E system is the largest computer system of its kind and, for climate modeling and fusion simulation, it is the fastest computer available. The Cray XT3 system is the most powerful unclassified system available to DOE and university researchers. It can deliver more than 25 trillion calculations per second, and has more than 10 trillion bytes of memory.

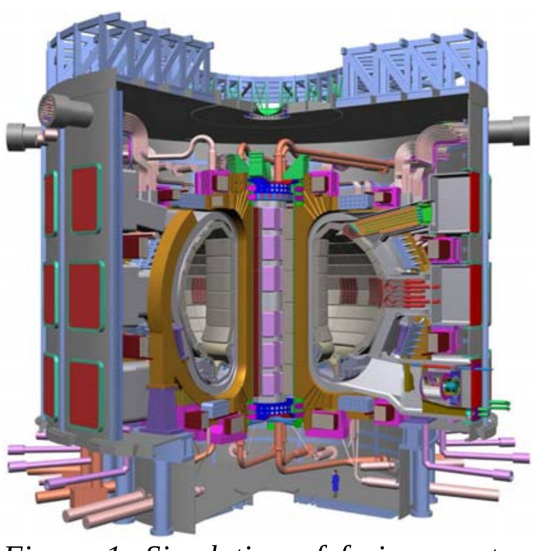

Figure 1. Simulation of fusion reactors at the LCF is critical to the nation's energy independence.

The LCF has an aggressive roadmap to sustain leadership for scientific computing.

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The plan will quadruple the performance of the Cray XT3 system in 2006 to 100 trillion operations per second. Our goal is to achieve 1,000 trillion operations per second in 2008, meeting the growing demand of scientists for faster, more powerful tools to achieve critically needed simulations that will enhance or replace more costly, less accurate experimental investigations.

In 2005, researchers were provided access to Leadership Computing Facility resources to initiate advanced studies in the areas of chemistry, combustion, fusion, astrophysics, and accelerator simulation (Figures 1 and 2). From calculations that now take weeks, rather than months or years, researchers are gaining new insight into the chemistry of extinction and re-ignition mechanisms, keys to developing combustors that use fuel efficiently and minimize harmful emissions.

Alternative energy source exploration is being aided by CCS investigations of the physics of turbulence and plasma behavior on the design of fusion power systems. This research is 10 times faster on vector versus non-vector processors, and the Leadership Computing Facility Cray X1E is the only vector system of its size in the United States that is available for open research.

The CCS is connected to major network hubs in Atlanta and Chicago, making this unique user facility accessible to academia, industry, and other laboratories (Figure 3). This network represents a truly world-class infrastructure, allowing the creation of on-demand, short or long-term dedicated channels at 10 gigabits per second or more for data traffic between the Leadership Computing Facility and DOE's UltraScience network and ESNET, NSF's Extensible Terascale Facility, Internet2, and National Lambda Rail, among others.

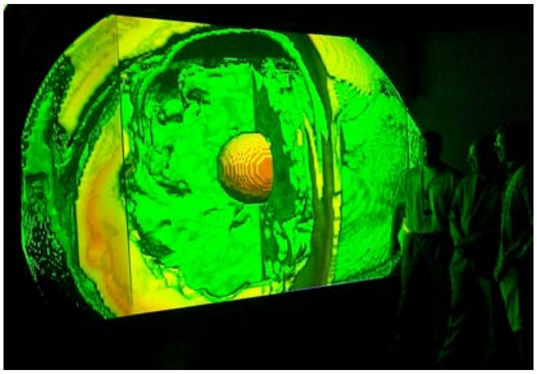

Figure 2. Simulation results of core collapse supernovae mechanisms from John Blondin, North Carolina State University, and Tony Mezzacappa, ORNL.

The network and physical infrastructure of the CCS is designed to expand with the demands of the scientific community, and is poised to support new systems that will enable leading-edge research. The exceptional combination of human and computer resources provides a significant advantage to users of the facility, and an opportunity for collaborative investigations.

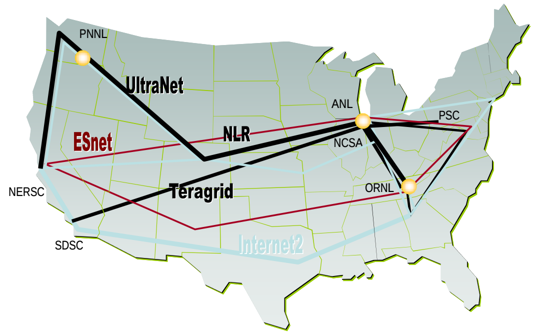

Figure 3. The CCS is connected to every major scientific and research network in the country.

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Largest ever AORSA Simulation

Fred Jaeger,* Don Batchelor, Oak Ridge National Laboratory

Summary

In August 2005, just weeks after the delivery of the final cabinets of ORNL's Cray XT3, researchers at the Center for Computational Sciences ran the largest plasma wave simulation for fusion based research.

The United States is one of the largest consumers of non-renewable energy resources, and the growth of third-world nations is greatly accelerating this depletion. Yet a virtually inexhaustible energy supply is tantalizingly close to us, and directly overhead.

"Researchers are acutely aware of earth's dwindling supplies of petroleum and other non-renewable energy sources. They have been trying for decades to reproduce the power of the sun, which is created by the fusion of small atoms under temperatures of millions of degrees Celsius to produce plasma," said Don Batchelor, head of the Plasma Theory Group in ORNL's Fusion Energy Division. "A major advantage of plasma energy, aside from its near-limitlessness, is that it is 'clean' and does not contribute to global climate change."

To utilize plasma energy, the U.S., Europe, and other nations have joined forces to develop ITER, a multi-billion dollar International Thermonuclear Experimental Reactor, by 2016. ITER's reactor uses magnetic fields to contain a roiling maelstrom of plasma, or gaseous particles, which comprise the 'fuel' for the fusion reaction.

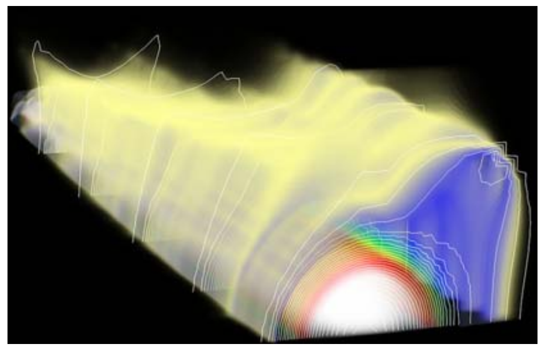

Figure 1. Velocity distribution function for ions heated by radio frequency (RF) waves in a tokamak plasma.

Cost-effective and efficient development and operation of ITER depend on the ability to simulate, understand and control the behavior of this plasma: its physics and optimal conditions that foster fusion. AORSA (All-Orders Spectral Algorithm) application, illuminates the behavior of plasma control waves (Figure 1).

"Using 3,072 processors, or about 60 percent, of the new Cray XT3 at ORNL's Center for Computational Sciences, we were able to run the largest, most-detailed simulation ever done of plasma control waves in a tokamak, the donut-shaped reactor that will eventually form the core of the multinational ITER reactor," said Fred Jaeger, the ORNL researcher who ran the

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simulation. "We were able to complete the simulations three to seven times faster than when we run the same application on another DOE high performance computing system." (Figure 2).

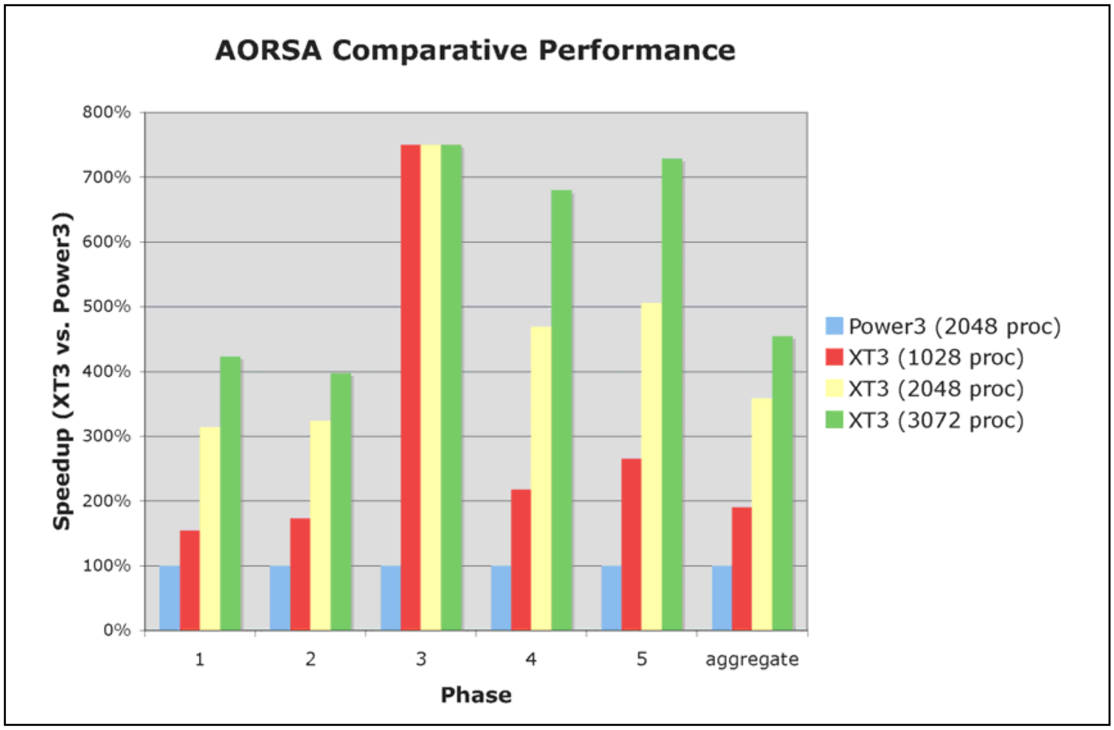

Figure 2. AORSA calculations.

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Combustion Simulation: Turbulent Nonpremixed Flames

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Summary

Advancing basic understanding of turbulent combustion and developing predictive combustion models are essential to deliver reliable data for manufacturer design of combustors and to limit hardware testing costs.

The Challenge

Combustion equipment that uses fuel efficiently and minimizes harmful emissions is essential to building a secure, sustainable energy infrastructure. Faced with stiff global competition and concern over harmful emissions, makers of combustion devices (e.g., internal combustion engines, power turbines, industrial furnaces) are challenged to improve the reliability, fuel efficiency, and emissions performance of their products. High-performance computing is an unmatched tool for advancing combustion science via predictive models that will revolutionize combustion equipment design and performance.

Understanding the mechanisms governing flame extinction and re-ignition in a turbulent environment is key to developing those models. In many common combustors, fuel and air are injected separately into the combustion chamber rather than being premixed. Therefore, fundamental questions about the combustion process revolve around the rate at which the fuel and air mix in the chamber. Rapid mixing produces rapid energy release, allowing the use of smaller combustion chambers and reducing emissions. However, above a critical level, rapid mixing and the associated turbulence can extinguish combustion in areas of the flame or even destabilize the entire flame. Extinguished fuel–air pockets that fail to reignite quickly are exhausted from the combustor, and abundant extinguished pockets that do not re-ignite can halt combustion altogether. Thus extinction adversely affects energy efficiency, emissions, and safety.

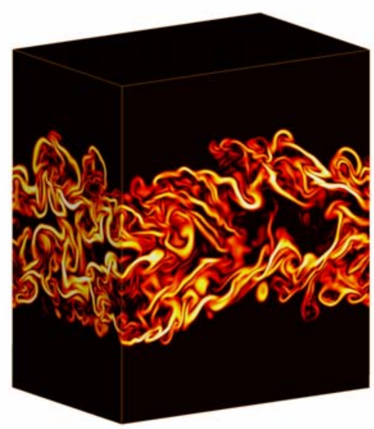

Figure 1. Scalar dissipation rate field (indication of local mixing intensity) in a turbulent plane jet flame.

Research at LCF

Researchers are using the Leadership Computing Facility (LCF) Cray X1E and XT3 massively parallel supercomputers to perform the first 3-dimensional turbulent direct numerical simulation (DNS) of a non-premixed $H_2/CO/N_2$–air flame with detailed chemistry to study extinction and re-ignition mechanisms. The DNS is part of a parametric study performed on three

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different Office of Science computing platforms: the IBM SP at NERSC (FY05 INCITE award), the HP Itanium-2 cluster at PNNL, and the ORNL CrayX1E and XT3.

The simulation is performed using the Sandia DNS code S3D, which has been used extensively to investigate fundamental turbulence-chemistry interactions. The chosen physical configuration corresponds to a temporally-evolving plane jet flame (Figure 1).

This DNS clarifies extinction and re-ignition mechanisms in a turbulent environment by including detailed chemistry (i.e., capable of fully representing burning and igniting chemical states), heat release, and realistic thermo-chemical properties. Unlike previous DNS studies, this one permits reignition to occur by either autoignition or flame propagation. Statistics will be obtained for the occurrence of the different modes of reignition as a function of key flow and flame parameters.

The resulting numerical benchmark data will complement a library of experimental flame data on non-premixed turbulent combustion. They will be shared with an international collaboration of researchers working to advance the predictive capability of combustion models. A key limitation in existing models is their inability to describe combustion phenomena involving coupling of finite-rate chemistry with turbulence. It is exactly this type of information that the DNS will provide.

How LCF Enables this Research

These simulations require millions of cpu-hours with between 50 and 500 million grid points on terascale computers. On the NLCF computers, it is possible to run the process in weeks rather than in months or years. To achieve the needed fidelity in a reasonable amount of processing time, it is advantageous to perform these simulations on a vector processing architecture (one that operates on a large array of values simultaneously, rather than on just a few values). Test runs have shown the DNS code S3D runs two times faster on the vector system than on a non-vector system. The Cray X1E is one of the only vector systems in the United States that is available for open research.

A production calculation using 100 million grid points had been performed on the LCF’s Cray X1E by the third quarter of FY 2005. The preliminary calculations indicate that both diffusivity and the strong interplay between reaction and diffusion in non-premixed flames affect mixing time scales. The findings underline the importance of considering the interplay of diffusion and reaction, particularly where strong finite-rate chemistry effects are involved. At present, highly resolved simulations of this sort are the only way to obtain this type of information.

Impact of Combustion Simulations

Advances in combustion device design have traditionally been incremental—making small changes from previous designs and then building hardware to test the results. This slow, costly approach is ill-suited to the challenges of modern manufacturing and global competition. Reliable, detailed computer modeling will enable designers to explore radical design changes and complex control strategies rapidly with limited need for hardware testing.

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Advanced Simulations of Plasma Microturbulence

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Summary

Fusion simulations at the Leadership Computing Facility (LCF) at Oak Ridge National Laboratory help drive the development of alternative, clean energy resources.

The Challenge

As worldwide demand for energy accelerates, and the reality of a finite petroleum supply asserts itself, the need for alternative energy sources is becoming acute. Scientists have long dreamed of harnessing fusion, the process that powers the sun and other stars, as a primary energy source. The capability to use fusion energy will revolutionize the energy system worldwide because fusion power plants will use abundant fuels available to all nations and will produce no greenhouse gas emissions, weapons materials, or hard-to-manage waste. Development of this secure, reliable, economically and environmentally sustainable energy source is one of the most important challenges of the 21st century.

Although fusion has been successfully demonstrated and has made continuous progress, it is still in the research stage, and fundamental questions still must be resolved. Realistic physics-based computer simulations are essential to fusion experimentation: they provide data that enable researchers to set up plasma systems to achieve the conditions required for fusion reactors, and they predict the effects experiments are likely to produce and whether such effects can be measured by the available instruments. Ultimately, the design of devices adequate for plasma confinement will depend on models of plasma behavior under realistic conditions. Plasma turbulence, internal roiling that accelerates the diffusion of particles and heat in the plasma, is an essential area of inquiry. Turbulence causes the plasma to lose the heat essential to maintaining fusion. Reliable modeling of turbulence is an indispensable step toward formulating strategies for controlling it.

Research at LCF

Researchers are using the Cray X1E supercomputer at the LCF to model the flow of charged particles in fusion plasmas to accurately simulate the evolution of turbulence over an extended period of time and show what is happening to particles in the plasma as turbulence occurs. The immediate objective is to significantly increase the number of particles modeled per cell of the simulation while keeping processing times manageable. Simulations target an improved understanding of why the turbulence level associated with key instabilities driven by the thermal gradient of the plasma can saturate at a lower level and at a faster rate when additional

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"nonlinear" terms are added to equations describing particle velocity.

These studies are being carried out at the LCF using the Gyrokinetic Toroidal Code (GTC), a particle-in-cell code for simulating complex microturbulence properties in fusion-grade plasmas. GTC is very actively involved in benchmark tests on advanced supercomputing platforms, and is the lead code in the DOE's SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas.

What Researchers will Achieve
Simulations conducted with a significantly higher number of particles provide a more highly resolved set of statistics for a more detailed, accurate picture of how particles behave in a turbulent plasma medium. These studies provide insights into (1) the extent to which inadequate statistical data have impacted the ability to realistically simulate the long-time evolution of plasma turbulence and (2) how the processes that govern particle velocity drive the turbulence to reach the steady state more rapidly.

How LCF Enables this Research
The larger of these simulations will model almost 4 billion particles. To achieve the needed simulation fidelity in a reasonable amount of processing time, the simulations must be performed on a vector processing system (one that operates on a large array of values simultaneously, rather than on just a few values). Previous test runs have demonstrated that GTC runs 10 times faster per processor on the Cray X1E's vector processors than on the non-vector machine currently used for production simulations. Since the Cray X1E is one of the only vector systems in the United States available for open research, its unique capabilities are essential to breakthrough research in fusion simulation.

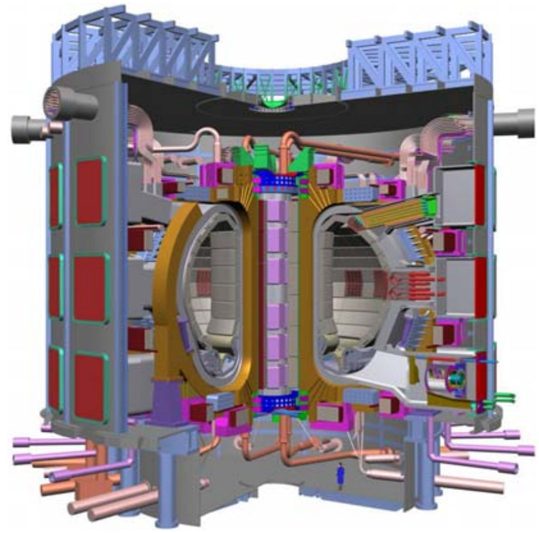

Figure 1. In June 2005, a site was selected for the International Thermonuclear Experiment Reactor (ITER), an international magnetic fusion research facility. Recognizing the promise of fusion energy, the U.S. Department of Energy Office of Science has named ITER its highest-priority scientific facility. To conduct experiments successfully in ITER, scientists require sophisticated fusion simulation tools.

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